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Cumulant expansion treatment of phonon contributions to the electron spectral function[1] S.M. STORY, J.J. KAS, University of Washington, M.J. VERSTRAETE, Université de Liège, J.J. REHR, University of Washington — We present an approach for calculations of phonon contributions to the electron spectral function at finite temerature based on cumulant expansion techniques. Our approach is based on a many–pole representation of the Eliashberg function for the electron–phonon interaction, calculations of the dynamical matrix using ABINIT [1], and an Einstein self–energy model [2]. The code has been implemented as part of a plug–in to ABINIT for calculations of various phonon properties, and is applicable to complex structures with several atoms per unit cell. Results are given for a number of systems and compared to those obtained with the GW approximation.

[1] X. Gonze et al., Computational Materials Science **25**, 478 (2002).
[2] A. Eiguren and C. Ambrosch–Draxl, Phys. Rev. Lett. **101**, 036402 (2008).

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